LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Title : SVOA CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.222 | 20 | 23 | 28 | rVB3 | 34731 | 44793 | 1.03% | 0.081% |
| 2 | 6.851 | 633 | 640 | 653 | rVB2 | 818148 | 1544933 | 35.69% | 2.792% |
| 3 | 7.010 | 661 | 667 | 678 | rVB | 620566 | 940874 | 21.74% | 1.701% |
| 4 | 7.204 | 691 | 700 | 712 | rBV | 833280 | 1325916 | 30.63% | 2.397% |
| 5 | 7.669 | 771 | 779 | 788 | rBV | 757602 | 1220971 | 28.21% | 2.207% |
| 6 | 8.375 | 893 | 899 | 913 | rVB | 1064299 | 1745960 | 40.34% | 3.156% |
| 7 | 8.822 | 968 | 975 | 985 | rBV | 848367 | 1418063 | 32.76% | 2.563% |
| 8 | 8.951 | 992 | 997 | 1009 | rVB3 | 39401 | 70790 | 1.64% | 0.128% |
| 9 | 9.539 | 1090 | 1097 | 1107 | rBV | 721609 | 1229976 | 28.42% | 2.223% |
| 10 | 10.075 | 1181 | 1188 | 1204 | rVB | 1104326 | 1906841 | 44.06% | 3.447% |
| 11 | 10.445 | 1244 | 1251 | 1261 | rBV | 1067208 | 1778767 | 41.10% | 3.215% |
| 12 | 10.592 | 1269 | 1276 | 1290 | rBV | 946043 | 1722253 | 39.79% | 3.113% |
| 13 | 13.133 | 1699 | 1708 | 1716 | rBV3 | 37074 | 61039 | 1.41% | 0.110% |
| 14 | 13.727 | 1803 | 1809 | 1813 | rBV | 2154084 | 2964224 | 68.49% | 5.358% |
| 15 | 13.774 | 1813 | 1817 | 1825 | rVB | 730209 | 1012453 | 23.39% | 1.830% |
| 16 | 14.004 | 1845 | 1856 | 1864 | rBV | 2291274 | 3403903 | 78.64% | 6.152% |
| 17 | 14.215 | 1885 | 1892 | 1897 | rBV | 129887 | 168941 | 3.90% | 0.305% |
| 18 | 14.310 | 1901 | 1908 | 1916 | rBV2 | 1545861 | 2368580 | 54.72% | 4.281% |
| 19 | 14.533 | 1940 | 1946 | 1956 | rBV | 593018 | 1075724 | 24.85% | 1.944% |
| 20 | 14.833 | 1994 | 1997 | 2002 | rVB6 | 34051 | 53880 | 1.24% | 0.097% |
| 21 | 15.168 | 2050 | 2054 | 2061 | rVB | 157801 | 202184 | 4.67% | 0.365% |
| 22 | 15.310 | 2072 | 2078 | 2089 | rVB | 2911472 | 4069237 | 94.02% | 7.355% |
| 23 | 15.445 | 2095 | 2101 | 2110 | rBV | 666399 | 1005273 | 23.23% | 1.817% |
| 24 | 15.551 | 2114 | 2119 | 2121 | rVV3 | 45650 | 64142 | 1.48% | 0.116% |
| 25 | 15.574 | 2121 | 2123 | 2128 | rVB5 | 37753 | 52345 | 1.21% | 0.095% |
| 26 | 16.033 | 2196 | 2201 | 2209 | rBV2 | 145499 | 234044 | 5.41% | 0.423% |
| 27 | 16.827 | 2331 | 2336 | 2339 | rBV | 81669 | 98173 | 2.27% | 0.177% |
| 28 | 17.062 | 2369 | 2376 | 2385 | rBV2 | 1874768 | 2588873 | 59.81% | 4.679% |
| 29 | 17.162 | 2386 | 2393 | 2402 | rBV2 | 2941104 | 4199917 | 97.03% | 7.591% |
| 30 | 17.568 | 2456 | 2462 | 2466 | rBV2 | 37916 | 52945 | 1.22% | 0.096% |
| 31 | 17.968 | 2524 | 2530 | 2540 | rBV | 474671 | 723477 | 16.72% | 1.308% |
| 32 | 19.097 | 2718 | 2722 | 2725 | rBV2 | 47238 | 64231 | 1.48% | 0.116% |
| 33 | 19.127 | 2725 | 2727 | 2737 | rVB9 | 34632 | 74857 | 1.73% | 0.135% |
| 34 | 19.250 | 2743 | 2748 | 2756 | rBV | 233132 | 345569 | 7.98% | 0.625% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Title : SVOA CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 19.462 | 2777 | 2784 | 2790 | rVV | 3117498 | 4328261 | 100.00% | 7.823% |
| 36 | 19.515 | 2790 | 2793 | 2797 | rVB3 | 55483 | 67454 | 1.56% | 0.122% |
| 37 | 19.986 | 2869 | 2873 | 2875 | rBV4 | 28972 | 44688 | 1.03% | 0.081% |
| 38 | 20.968 | 3036 | 3040 | 3048 | rBV | 492495 | 708783 | 16.38% | 1.281% |
| 39 | 21.174 | 3072 | 3075 | 3078 | rBV4 | 47343 | 52679 | 1.22% | 0.095% |
| 40 | 21.250 | 3083 | 3088 | 3095 | rBV | 1723245 | 2312697 | 53.43% | 4.180% |
| 41 | 21.368 | 3105 | 3108 | 3112 | rVB3 | 44252 | 58597 | 1.35% | 0.106% |
| 42 | 22.427 | 3284 | 3288 | 3295 | rVB | 276092 | 390022 | 9.01% | 0.705% |
| 43 | 23.333 | 3435 | 3442 | 3452 | rBV2 | 1784951 | 3565840 | 82.39% | 6.445% |
| 44 | 23.474 | 3459 | 3466 | 3475 | rBV | 1064307 | 2017627 | 46.62% | 3.647% |
| 45 | 25.891 | 3869 | 3877 | 3890 | rVB5 | 690963 | 1945468 | 44.95% | 3.516% |

Sum of corrected areas: 55326264

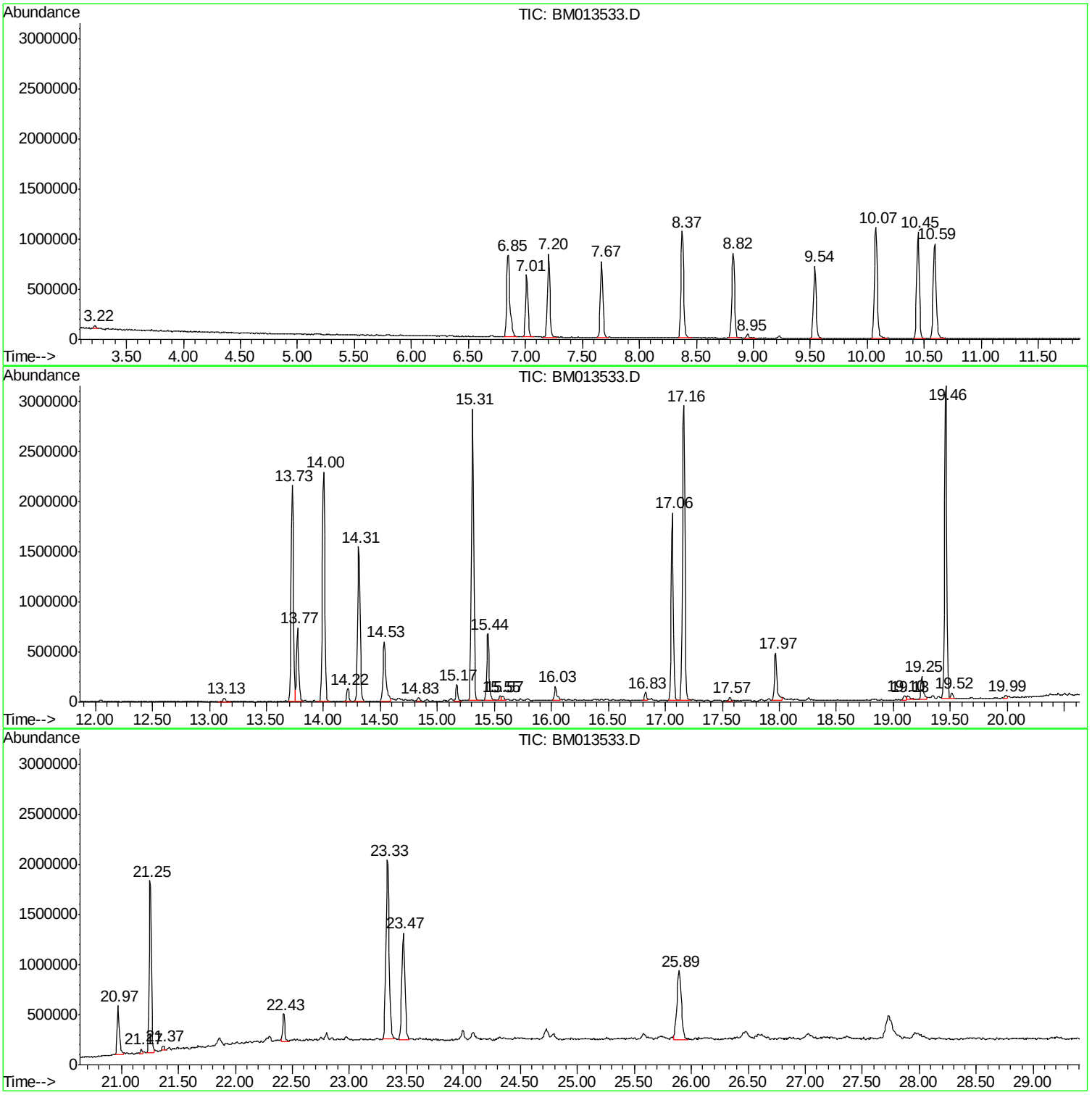
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

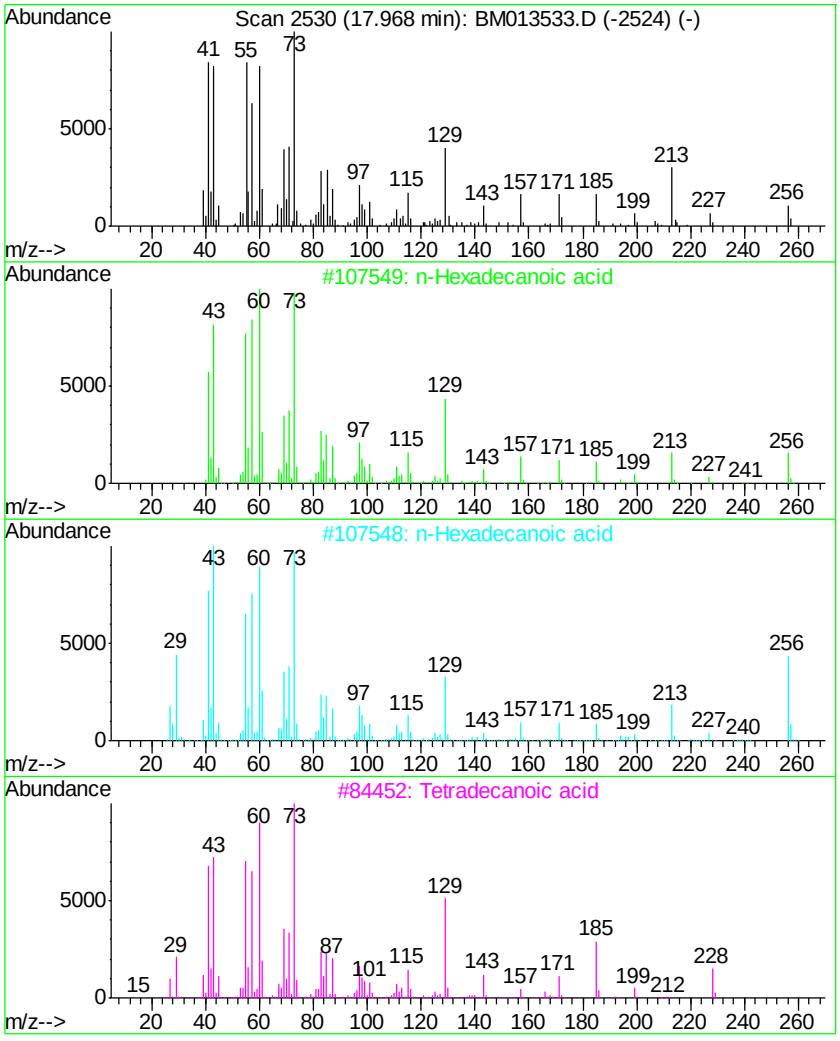
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

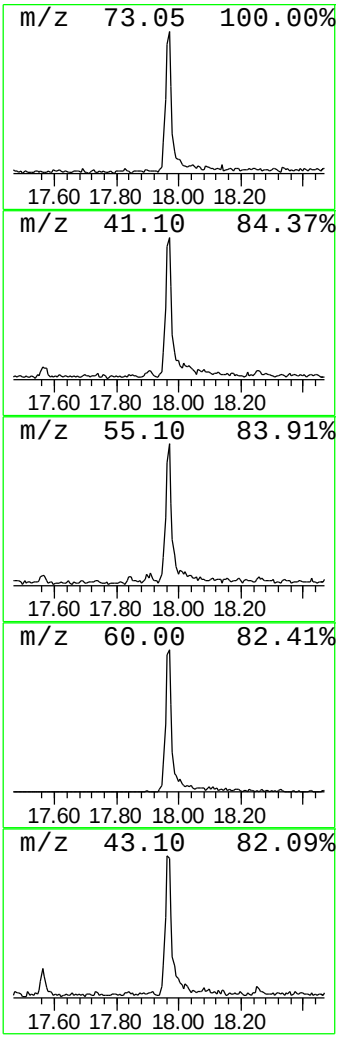
**********

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.97 | 5.59 ng/ul | 723477 | Phenanthrene-d10 | 17.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 95 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 92 |



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

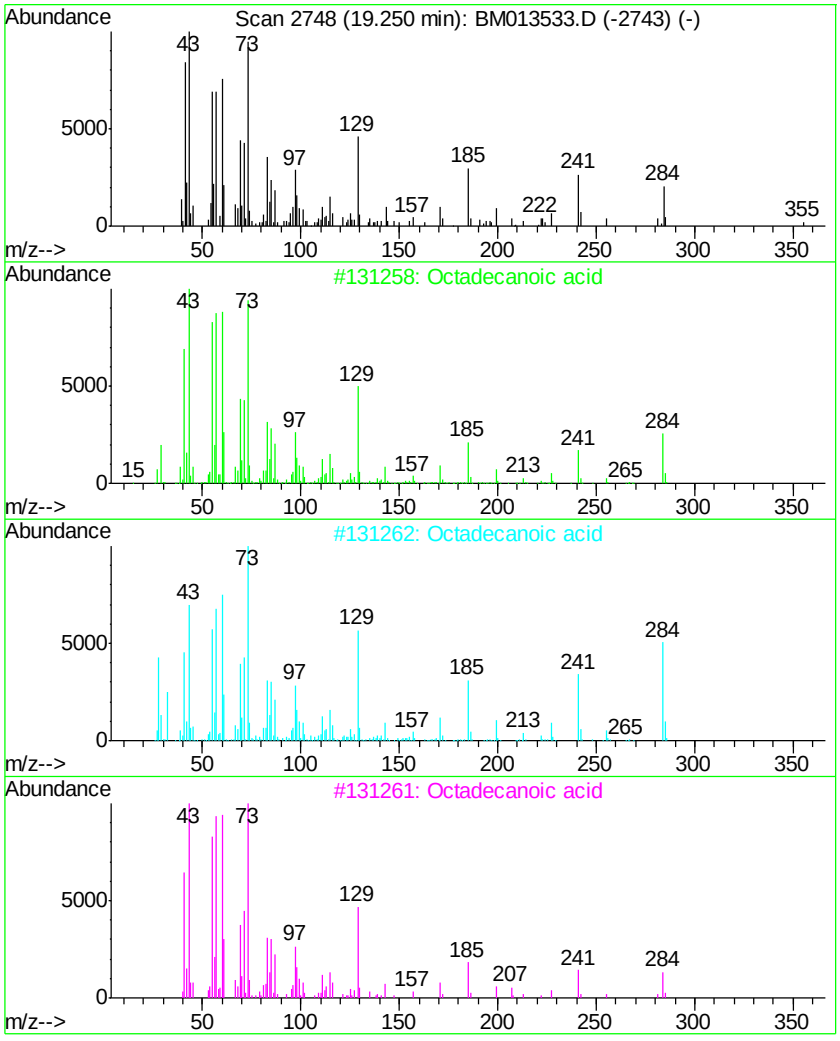
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

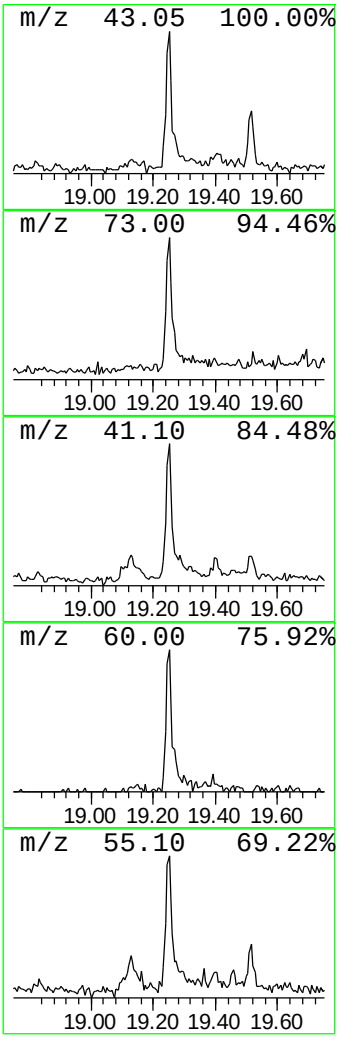
**********

Peak Number 2 Octadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.25 | 2.99 ng/ul | 345569 | Chrysene-d12 | 21.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 98 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 94 |
| 5 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 93 |



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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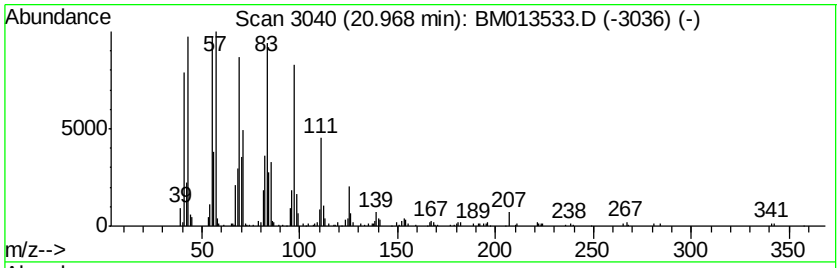
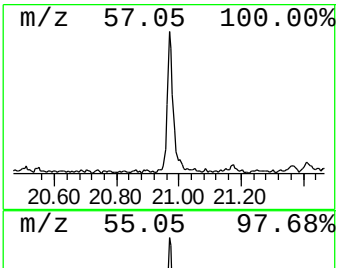
Peak Number 3 1-Heneicosanol Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.97 | 6.13 ng/ul | 708783 | Chrysene-d12 | 21.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |
| 4 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 91 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 90 |



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

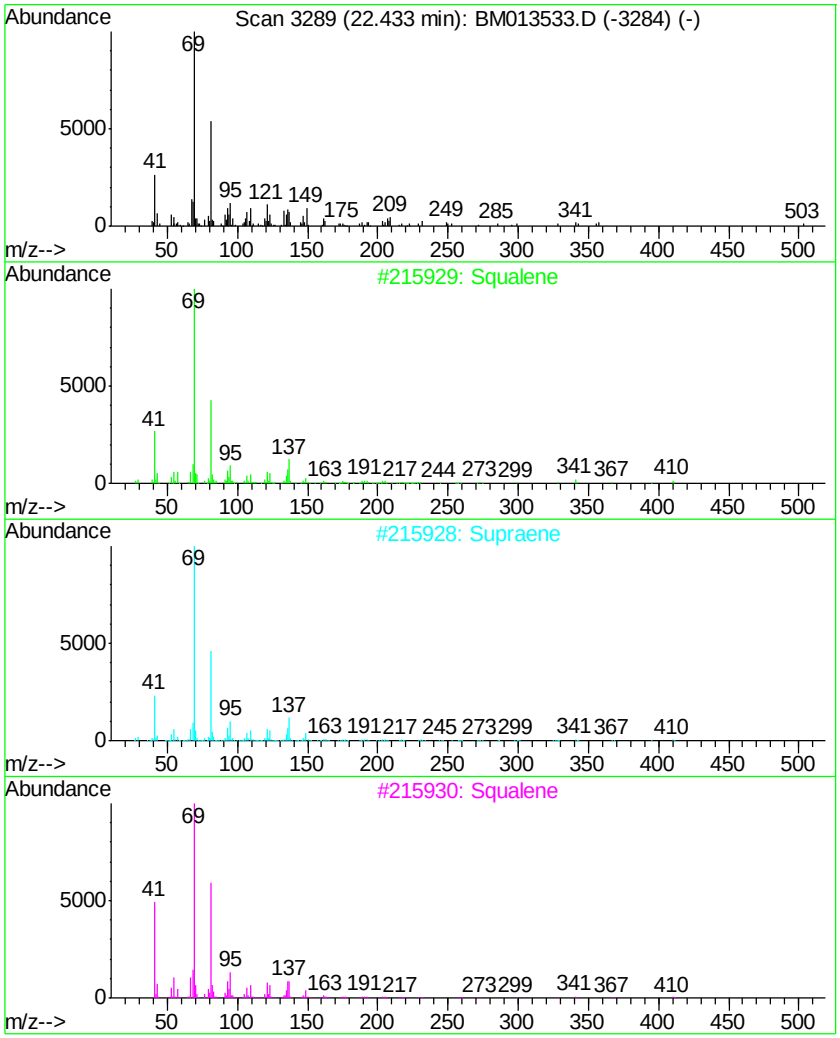
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

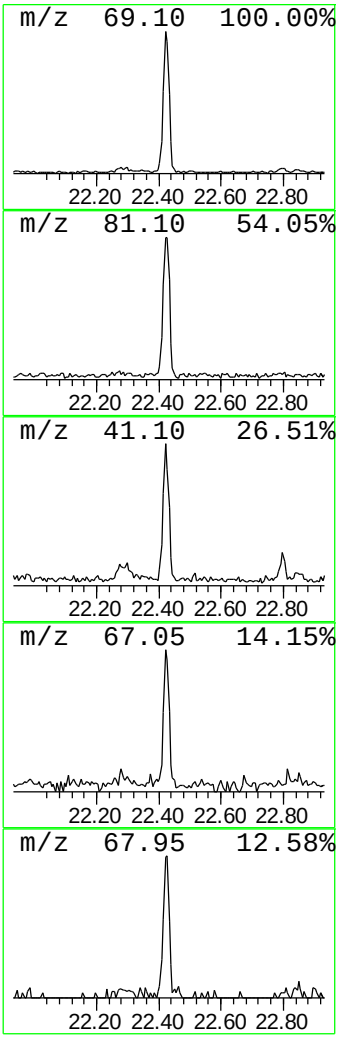
**********

Peak Number 4 Squalene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.43 | 3.87 ng/ul | 390022 | Perylene-d12 | 23.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 83 |
| 3 | Squalene | 410 | C30H50 | 000111-02-4 | 83 |
| 4 | Squalene | 410 | C30H50 | 000111-02-4 | 80 |
| 5 | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66 | 000502-62-5 | 72 |



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Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

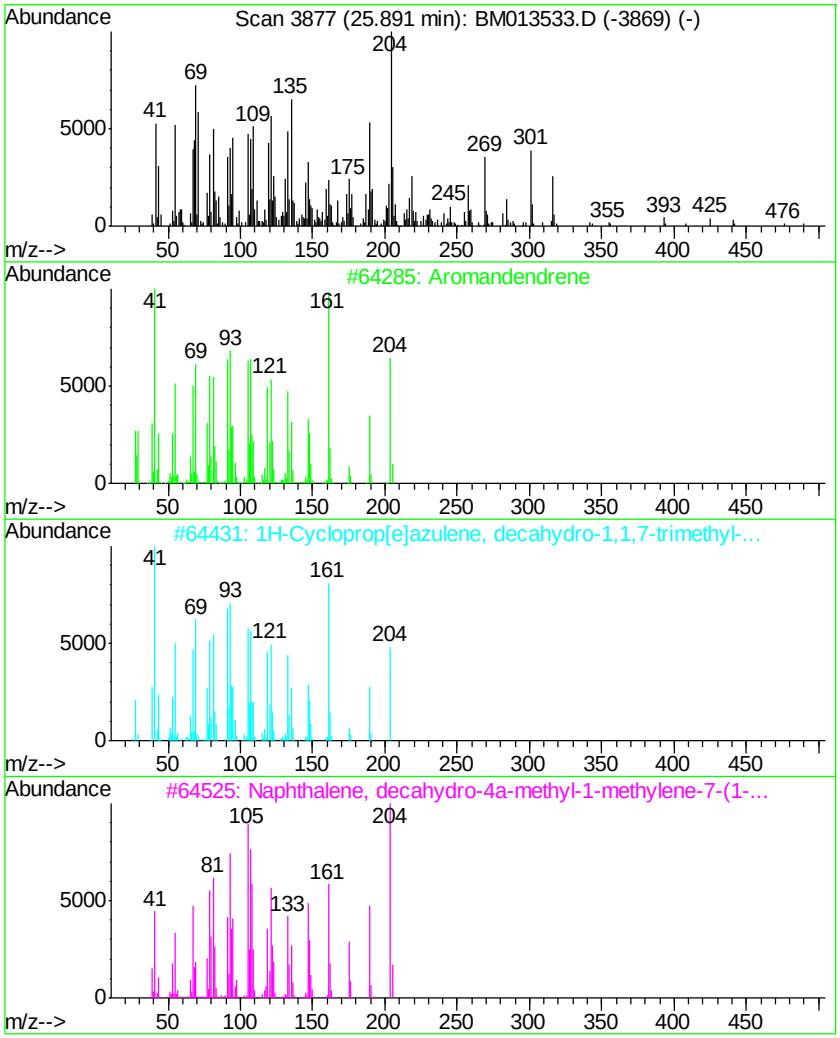
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

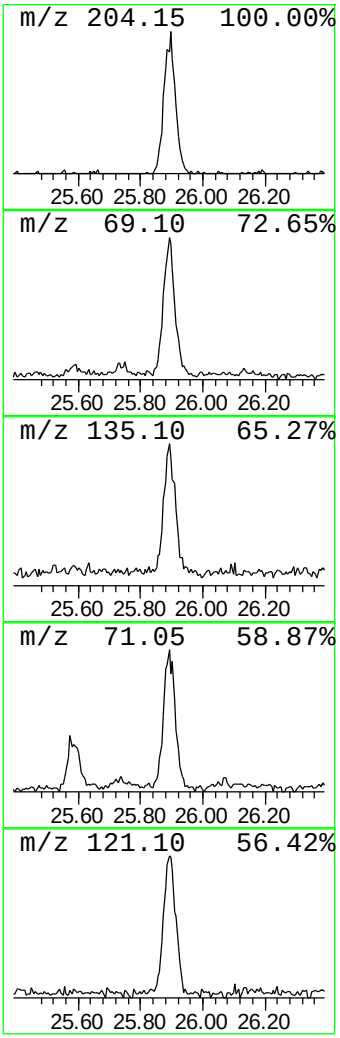
**********

Peak Number 5 Aromandendrene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 25.89 | 19.28 ng/ul | 1945470 | Perylene-d12 | 23.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Aromandendrene | 204 | C15H24 | 000489-39-4 | 78 |
| 2 | 1H-Cycloprop[e]azulene, decahydr... | 204 | C15H24 | 072747-25-2 | 58 |
| 3 | Naphthalene, decahydro-4a-methyl... | 204 | C15H24 | 017066-67-0 | 52 |
| 4 | Guaia-3,9-diene | 204 | C15H24 | 000489-83-8 | 50 |
| 5 | 1H-Cycloprop[e]azulene, 1a,2,3,4... | 204 | C15H24 | 000489-40-7 | 50 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122617\
Data File : BM013533.D
Acq On : 26 Dec 2017 14:15
Operator : SJ/JU
Sample : I7046-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** C0FL3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM113017.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| n-Hexadecanoic acid | 17.97 | 5.6 | ng/ul | 723477 | 4 | 17.06 | 2588870 | 20.0 |
| Octadecanoic acid | 19.25 | 3.0 | ng/ul | 345569 | 5 | 21.26 | 2312700 | 20.0 |
| 1-Heneicosanol | 20.97 | 6.1 | ng/ul | 708783 | 5 | 21.26 | 2312700 | 20.0 |
| Squalene | 22.43 | 3.9 | ng/ul | 390022 | 6 | 23.47 | 2017630 | 20.0 |
| Aromandendrene | 25.89 | 19.3 | ng/ul | 1945470 | 6 | 23.47 | 2017630 | 20.0 |